

Panel on Future of Computational Infrastructures

Panel Organizer: Dr. Esther Takeuchi, BESAC

Moderator: Abbas Ourmazd, BESAC

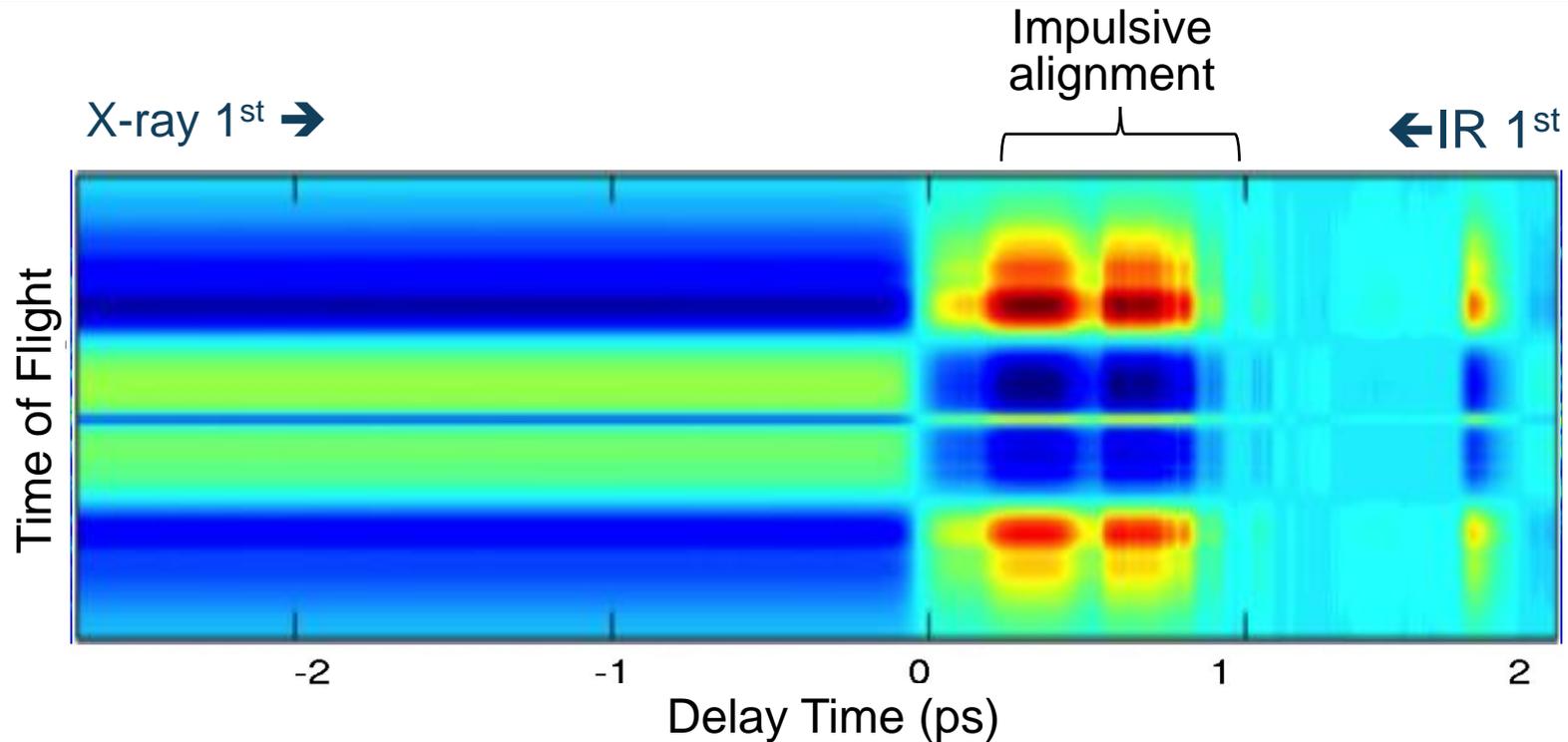


U.S. DEPARTMENT OF
ENERGY

Office of
Science



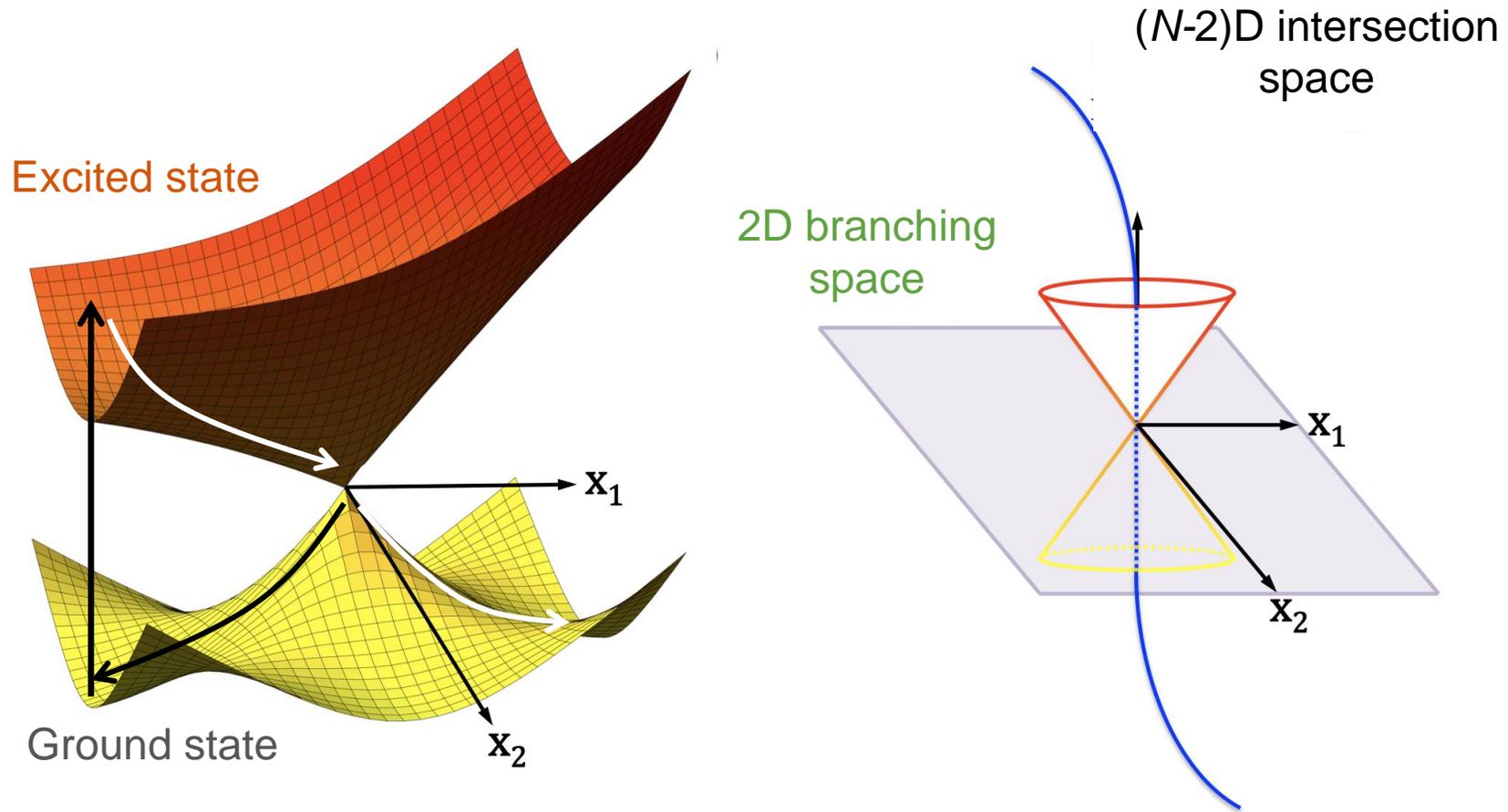
POWER OF AI/ML: FEMTOSECOND DYNAMICS FROM “LOUSY DATA”



Single femtosecond structural dynamics
Extracted from 98% incomplete, noisy data
Recorded with 280fs timing uncertainty
Fung, Hosseinizadeh et al., *Nature* (2016), (2021)



PHOTON-INDUCED ULTRAFAST STRUCTURAL DYNAMICS

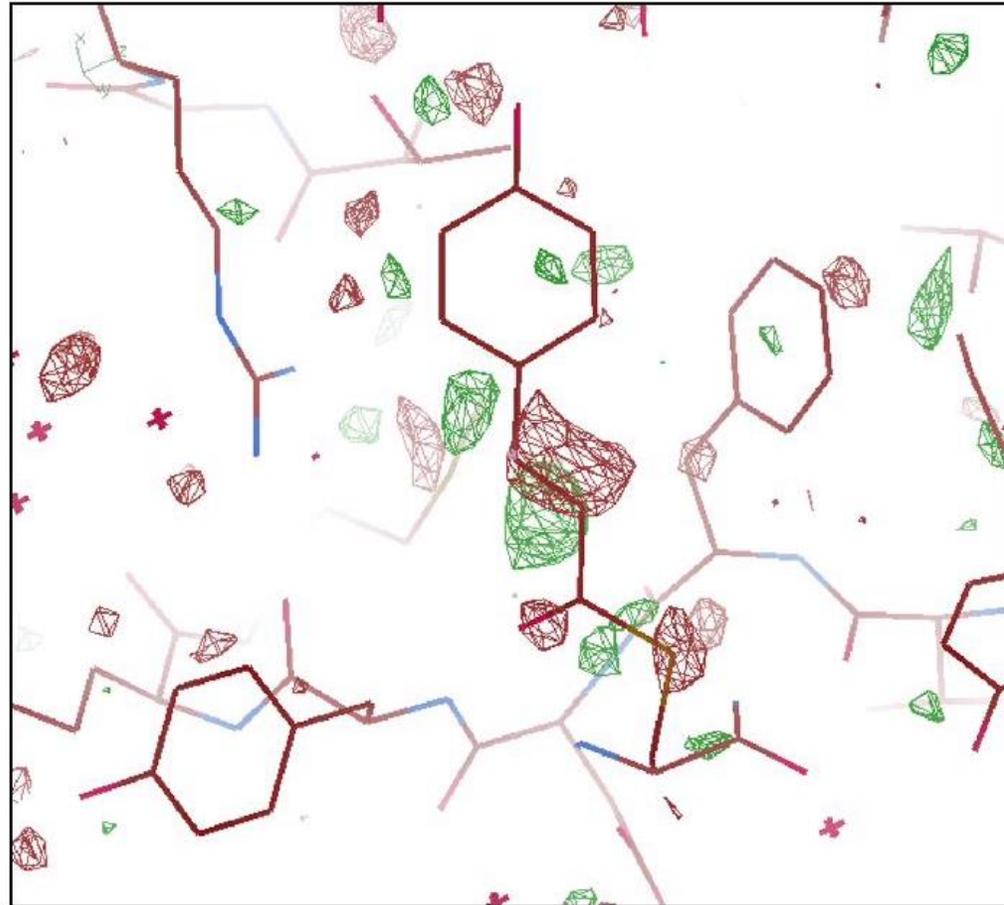
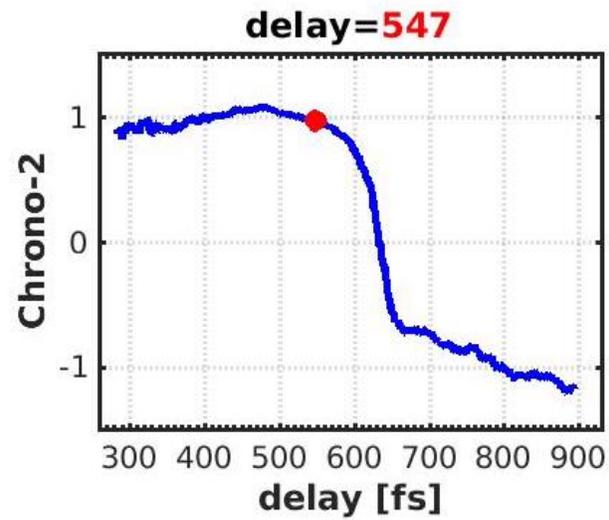




CONICAL INTERSECTION: THE MOVIE

Hosseinizadeh et al, *Nature*, 2021

Time resolution: ~ 1 fs
Spatial resolution: ~ 1.6 Å





POWER IN COMBINATION

Combine capabilities of multiple facilities

Tackle science problems currently out of reach
Whole greater than sum of the parts

Combine impact of Exascale Computing & Integrated Research Infrastructure

Computational infrastructure for the future

Combine data collection & data analysis (AI/ML)

E.g., Autonomous data collection enhances impact of facilities
Data analysis to take home knowledge, not only data



EXPERT PANEL MEMBERS

Dr. Eli DART

Network engineer and acting group leader in the ESnet Science Engagement Group.

Uses advanced networking to improve scientific productivity and science outcomes for the DOE science facilities.

Over 20 years experience in network architecture, design, engineering, performance, and security in scientific and research environments. Primary professional interests are high-performance architectures and effective operational models for networks



EXPERT PANEL MEMBERS

Dr. Barbara HELLAND

Associate Director of the Office of Science's Advanced Scientific Computing Research (ASCR) program

Leading Department's Exascale Computing Initiative to deliver a capable Exascale ecosystem

Recently received a 2022 HPCwire Editor's choice award for "Outstanding Leadership in HPC"



EXPERT PANEL MEMBERS

Mr. Nicholas SCHWARZ

Principal Computer Scientist at Argonne National Laboratory

Lead for scientific software and data management at the Advanced Photon Source

Co-organizer of regular workshop on Extreme-Scale Experiment-in-the-Loop Computing as a part of the annual SC conference series

Most recently served as member of the DOE/SC Integrated Research Infrastructure Architecture Blueprint Activity's Leadership Group



REQUEST

Only clarification questions between panel presentations

Other questions, comments, discussions *after* all panel member presentations



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